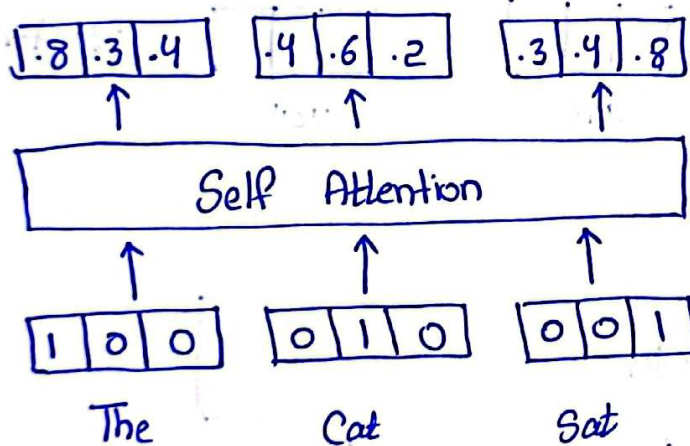


→ Self-Attention

Self-attention, also known as scaled dot-product attention, is a crucial mechanism in the transformer architecture that allows the model to weigh the importance of different tokens in the input sequence relative to each other.

> Idea



> Steps

1) Inputs

Q: Queries

K: Keys

V: Values

Model → Q, K, V

0

• Query Vector (Q)

Query vector represent the token for which we are calculating the attention. They help determine the importance of other tokens in the context of current token

Importance

↳ Focus Determination

Queries help the model to decide which parts of the sequence to focus on for each specific token. By calculating the dot product between a query vector (Q) and all key vectors (K), the model assesses how much attention to give to each token relative to the current token

↳ Contextual Understanding

Queries contribute to understanding the relationship between the current token and the rest of the sequence, which is essential for capturing dependencies and context.

- Key Vectors (K):

Key vectors represent all the tokens in the sequence and are used to compare with the query vectors to calculate attention scores.

Importance

└ Relevance Measurement

Keys are compared with queries to measure the relevance or compatibility of each token with the current token. This comparison helps in determining how much attention each token should have.

└ Information Retrieval

Keys play a critical role in retrieving the most relevant information from the sequence by providing a basis for the attention mechanism to compute similarity scores.

• Value Vectors (V):

Value vectors hold the actual information that will be aggregated to form the output of the attention mechanism.

Importance

└ Information Aggregation

Values contain the data that will be weighted by the attention scores. The weighted sum of values forms the output of the self-attention mechanism, which is then passed on to the next layers in the network.

└ Context Preservation

By weighting the values according to the attention scores, the model preserves and aggregates relevant context from the entire sequence, which is crucial for tasks like translation, summarization and more.

• Example

Input sequence = ["The", "cat", "Sat"]

Embedding size = 4 dimensions

$Q, K, V = 4$ dimensions

① Token Embeddings

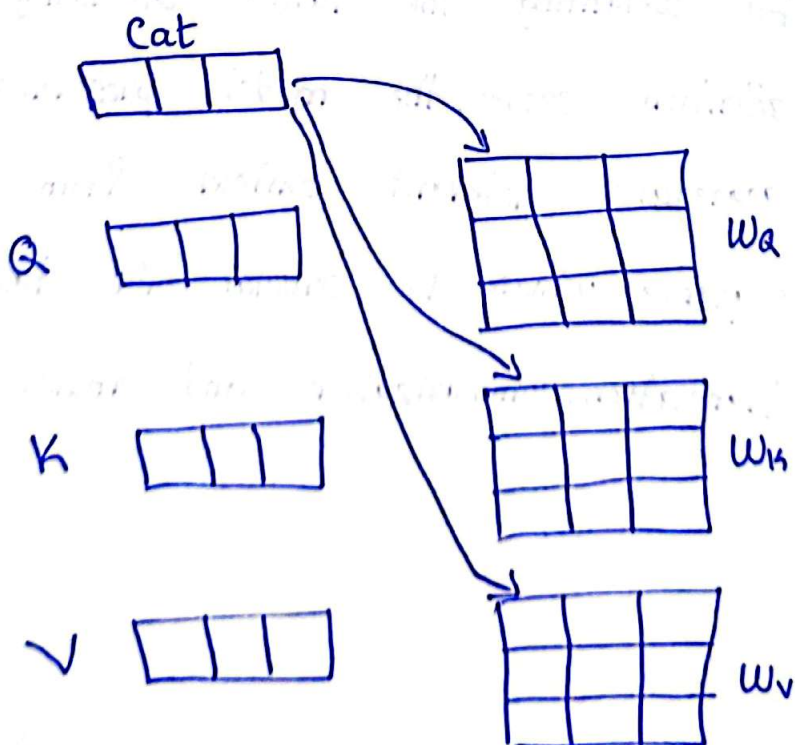
$$E_{\text{The}} = [1, 0, 1, 0]$$

$$E_{\text{cat}} = [0, 1, 0, 1]$$

$$E_{\text{Sat}} = [1, 1, 1, 1]$$

② Linear Transformation

We create Q, K, V by multiplying the embeddings by learned weight matrices: W_Q, W_K, W_V



$$W_Q = W_K = W_V = I$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$Q_{The} = E_{The} \cdot W_Q$$

$$Q_{The} = \begin{bmatrix} 1 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 1 & 0 \end{bmatrix}$$

$$K_{The} = \begin{bmatrix} 1 & 0 & 1 & 0 \end{bmatrix} \quad \therefore E_{The} \cdot W_K$$

$$V_{The} = \begin{bmatrix} 1 & 0 & 1 & 0 \end{bmatrix} \quad \therefore E_{The} \cdot W_V$$

$$1- Q_{The} = K_{The} = V_{The} = \begin{bmatrix} 1 & 0 & 1 & 0 \end{bmatrix}$$

$$2- Q_{cat} = K_{cat} = V_{cat} = \begin{bmatrix} 0 & 1 & 0 & 1 \end{bmatrix}$$

$$3- Q_{sat} = K_{sat} = V_{sat} = \begin{bmatrix} 1 & 1 & 1 & 1 \end{bmatrix}$$

③ Compute Attention Scores

For token = the

$$\text{Score}(Q_{The}, K_{The}) = \begin{bmatrix} 1 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 1 & 0 \end{bmatrix}^T = 2$$

$$\text{Score}(Q_{The}, K_{cat}) = \begin{bmatrix} 1 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 & 1 \end{bmatrix}^T = 0$$

$$\text{Score}(Q_{The}, K_{sat}) = \begin{bmatrix} 1 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 & 1 \end{bmatrix}^T = 2$$

For token = cat

$$\text{Score}(Q_{\text{cat}}, K_{\text{The}}) = [0 \ 1 \ 0 \ 1][1 \ 0 \ 1 \ 0]^T = 0$$

$$\text{Score}(Q_{\text{cat}}, K_{\text{cat}}) = [0 \ 1 \ 0 \ 1][0 \ 1 \ 0 \ 1]^T = 2$$

$$\text{Score}(Q_{\text{cat}}, K_{\text{sat}}) = [0 \ 1 \ 0 \ 1][1 \ 1 \ 1 \ 1]^T = 2$$

For token = sat

$$\text{Score}(Q_{\text{sat}}, K_{\text{The}}) = [1 \ 1 \ 1 \ 1][1 \ 0 \ 1 \ 0]^T = 2$$

$$\text{Score}(Q_{\text{sat}}, K_{\text{cat}}) = [1 \ 1 \ 1 \ 1][0 \ 1 \ 0 \ 1]^T = 2$$

$$\text{Score}(Q_{\text{sat}}, K_{\text{sat}}) = [1 \ 1 \ 1 \ 1][1 \ 1 \ 1 \ 1]^T = 4$$

④ Scaling

We take the scores and scale down by dividing the scores by the square root of dimensions of key vector

$$\begin{aligned} d_k &= \sqrt{4} \\ &= 2 \end{aligned}$$

Scaling in attention mechanism is crucial to prevent the dot product from growing too large

Problems:

- 1- Gradient Exploding
- 2- Softmax Saturation

Example without scaling

$$Q = [2 \ 3 \ 4 \ 1] \quad K_1 = [1 \ 0 \ 1 \ 0] \quad K_2 = [0 \ 1 \ 0 \ 1]$$

$$Q \cdot K_1^T = 2 \times 1 + 3 \times 0 + 4 \times 1 + 1 \times 0 = 6$$

$$Q \cdot K_2^T = 2 \times 0 + 3 \times 1 + 4 \times 0 + 1 \times 1 = 4$$

$$\text{Score} : [6, 4]$$

$$\begin{aligned} \text{Softmax}([6, 4]) &= \left[\frac{e^6}{e^6 + e^4}, \frac{e^4}{e^6 + e^4} \right] \\ &= \left[\frac{e^6}{e^6(1 + e^{-2})}, \frac{e^4}{e^4(e^2 + 1)} \right] \\ &= \left[\frac{1}{1 + e^{-2}}, \frac{1}{e^2 + 1} \right] \approx [0.88, 0.12] \\ &\quad \text{difference is huge} \end{aligned}$$

Most of the attention weights are assigned to the first key vector

Example with Scaling

$$\text{Score} : [6, 4] \Rightarrow \text{Scale} \Rightarrow \left[\frac{6}{2}, \frac{4}{2} \right] = [3, 2]$$

$$\text{Softmax}([3, 2]) = \left[\frac{e^3}{e^3 + e^2}, \frac{e^2}{e^3 + e^2} \right] = \left[\frac{e^3}{e^3(1 + e^{-1})}, \frac{e^2}{e^2(e + 1)} \right]$$

$$= \left[\frac{1}{1 + e^{-1}}, \frac{1}{e + 1} \right] \approx [0.73, 0.27]$$

Distance is less
difference

④ Scaling Cont.

for token = the

$$\text{Scaled-score}(Q_{\text{the}}, K_{\text{the}}) = 2/2 = 1$$

$$\text{Scaled-score}(Q_{\text{the}}, K_{\text{cat}}) = 0/2 = 0$$

$$\text{Scaled-score}(Q_{\text{the}}, K_{\text{sat}}) = 2/2 = 1$$

for token = cat

$$\text{Scaled-score}(Q_{\text{cat}}, K_{\text{the}}) = 0/2 = 0$$

$$\text{Scaled-score}(Q_{\text{cat}}, K_{\text{cat}}) = 2/2 = 1$$

$$\text{Scaled-score}(Q_{\text{cat}}, K_{\text{sat}}) = 2/2 = 1$$

for token = sat

$$\text{Scaled-score}(Q_{\text{sat}}, K_{\text{the}}) = 2/2 = 1$$

$$\text{Scaled-score}(Q_{\text{sat}}, K_{\text{cat}}) = 2/2 = 1$$

$$\text{Scaled-score}(Q_{\text{sat}}, K_{\text{sat}}) = 4/2 = 2$$

⑤ Apply Softmax

$$\text{Attention Weight}_{\text{the}} = \text{Softmax}([1, 0, 1]) = [0.42, 0.15, 0.42]$$

$$\text{Attention Weight}_{\text{cat}} = \text{Softmax}([0, 1, 1]) = [0.15, 0.42, 0.42]$$

$$\text{Attention Weight}_{\text{sat}} = \text{Softmax}([1, 1, 2]) = [0.21, 0.21, 0.58]$$

⑥ Weighted Sum of Values

Multiply attention weights to corresponding value vector

$$\begin{aligned}\text{Output}_{(\text{The})} &= 0.42 \times V_{\text{The}} + 0.15 \times V_{\text{cat}} + 0.42 \times V_{\text{sat}} \\ &= 0.42[1 \ 0 \ 1 \ 0] + 0.15[0 \ 1 \ 0 \ 1] + 0.42[1 \ 1 \ 1 \ 1] \\ &= [0.42 \ 0 \ 0.42 \ 0] + [0 \ 0.15 \ 0 \ 0.15] + \\ &\quad [0.42 \ 0.42 \ 0.42 \ 0.42] \\ &= [0.84 \ 0.57 \ 0.84 \ 0.57]\end{aligned}$$

$$[1 \ 0 \ 1 \ 0] \Rightarrow \text{Self-Attention} \Rightarrow [0.84 \ 0.57 \ 0.84 \ 0.57]$$

$$\begin{aligned}\text{Output}_{(\text{cat})} &= 0.15 \times V_{\text{The}} + 0.42 \times V_{\text{cat}} + 0.42 \times V_{\text{sat}} \\ &= 0.15[1 \ 0 \ 1 \ 0] + 0.42[0 \ 1 \ 0 \ 1] + 0.42[1 \ 1 \ 1 \ 1] \\ &= [0.15 \ 0 \ 0.15 \ 0] + [0 \ 0.42 \ 0 \ 0.42] + [0.42 \ 0.42 \ 0.42 \ 0.42] \\ &= [0.57 \ 0.84 \ 0.57 \ 0.84]\end{aligned}$$

$$\begin{aligned}\text{Output}_{(\text{sat})} &= 0.21[1 \ 0 \ 1 \ 0] + 0.21[0 \ 1 \ 0 \ 1] + 0.58[1 \ 1 \ 1 \ 1] \\ &= [0.21 \ 0 \ 0.21 \ 0] + [0 \ 0.21 \ 0 \ 0.21] + [0.58 \ 0.58 \ 0.58 \ 0.58] \\ &= [0.79 \ 0.79 \ 0.79 \ 0.79]\end{aligned}$$